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Sensitivity analysis when model outputs are functions

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Abstract

When outputs of computational models are time series or functions of other continuous variables like distance, angle, etc., it can be that primary interest is in the general pattern or structure of the curve. In these cases, model sensitivity and uncertainty analysis focuses on the effect of model input choices and uncertainties in the overall shapes of such curves. We explore methods for characterizing a set of functions generated by a series of model runs for the purpose of exploring relationships between these functions and the model inputs.

Keywords: Functional sensitivity analysis; Functional data analysis; Basis functions

1. Introduction

The outputs of computational models are often time series or functions of other continuous variables like distance, angle, etc. Following Campbell [1], we propose that sensitivity analysis of such outputs be carried out by means of an expansion of the functional output in an appropriate functional coordinate system, i.e., in terms of an appropriate set of basis functions, followed by sensitivity analysis of the coefficients of the expansion using any standard method. The principal new problem, therefore, is choosing an appropriate coordinate system in which to apply the selected sensitivity analysis methods. We consider both predefined basis sets and data-adaptive basis sets, with their associated advantages and disadvantages. We devote only passing mention to some related but important problems, such as increasing the interpretability of the results by appropriate preprocessing of the functional outputs (in particular, alignment or registration of curves), and by enforcing some degree of smoothness when data-adaptive bases are used.

We will use a simple made-up example for explaining ideas. Fig. 1 shows a sample of curves generated by varying the four parameters, a, b, c and d in the "model"

$$f(\theta) = 10 + a \exp\left(-\frac{(\theta-b)^2}{K_1 a^2 + c^2}\right) + (b+d)\exp(K_2 a\theta). \tag{1}$$

We interpret these functions as model output from a problem where the independent variable θ is a polar angle ranging from -90° to 90°. The model was run 81 times, using a complete 3^4 factorial design for the four input parameters.

In analyzing this "model output", we are typically less interested in what affects the values at, say, 45° than in questions such as: What shifts the curves up and down or moves them left or right? What makes the central peak wider or narrower? What makes the right-hand tail higher or lower? We could, of course, pick some appropriate functionals for answering these questions. The last, for example, we might address by examining the sensitivity of the values at 90° to the four input parameters. In order to address questions such as peak width, we could devise some surrogate measurement that could be computed on each curve and then study its sensitivity to the input parameters. However, such choices are highly problem specific.

2. Transforming functional data

It might seem natural to regard functions provided on a grid of T points as T-dependent variables for the purpose of sensitivity analysis. However, this approach can be unsatisfactory for many reasons:

- The T variables are highly correlated with one another, so this natural coordinate system is inefficient for

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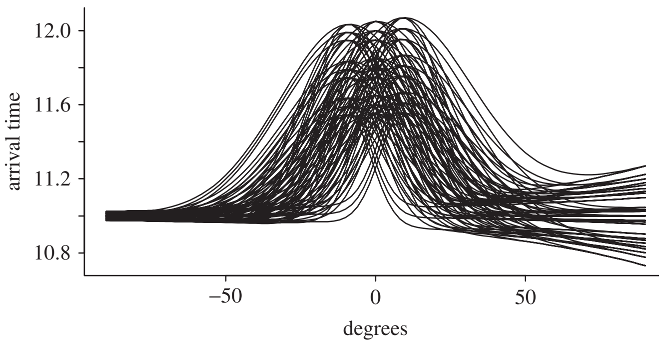

Fig. 1. Functional output from 81 runs of the example model.

statistical methods like discriminant analysis, sensitivity analysis, or almost anything other than multivariate statistical methods. Results are redundant from one value of θ to another.

- The pointwise results can be difficult to interpret for the underlying physical or modeling problem. In particular, information about the global functioning of the model or physical system contained in such curve features as location, scale and phase shifts, as well as in localized fluctuations including tail behavior, cannot generally be extracted from individual univariate analyses.
- Even though the data are the output of a computer model, the different runs may not have generated outputs at the same times or points θ. Alternatively, identical model output times may not be physically comparable because, as a function of the input parameters, the modeled process may be evolving faster in one run than another. So, we may need to register the output curves (rescale time) in some physically more interpretable manner before proceeding with analysis.

All of these problems can be addressed by transforming the functional output in one way or another. For sensitivity analysis, the most useful approach is expanding the output functions in terms of some basis functions (after rescaling time, if necessary) and then applying the statistical method of interest—in our case, a sensitivity analysis method—to the coefficients of that expansion. Different types of bases can be considered. There are familiar, predefined bases such as Legendre polynomials or other orthogonal polynomials, trigonometric functions, Haar functions, or wavelet bases. Adaptive basis functions include principal components and partial least-squares (PLS) components. Ramsay and Silverman [2] provide a detailed treatment of functional data analysis methodology. In the remainder of this section, we highlight the techniques that are directly relevant to the application of Section 1.

If the columns of $\Phi_{T\times K}$ ($K\leqslant T$) are a proposed set of basis functions, then the original functional output from N model runs, an $N\times T$ matrix Y, can be rewritten as

$$Y-\bar{Y}\approx H\Phi^{\mathrm{T}}, \tag{2}$$

where $\bar{Y}=N^{-1}11^{\mathrm{T}}Y$ with 1 the N-vector of ones, or

$$y_i(t)-\bar{y}(t)\approx\sum_{k=1}^{K}h_{ik}\varphi_k(t)\quad\text{for }1\leqslant i\leqslant N,$$

where the mean function $\bar{y}(t)$ is computed as the mean of the $y_i(t)$ for each t. Equality holds in (2) if and only if the row space of $Y-\bar{Y}$ is a subspace of the column space of Φ.

Most standard basis systems are orthonormal. For example, the Legendre polynomials are orthonormal with respect to Lebesgue measure on $[-1, 1]$. But the Legendre polynomials in $\sin(\theta)$, which are used in the example below, are not orthonormal with respect to ordinary Lebesgue measure $d\theta$, but only with respect to a weighted measure $\cos\theta\, d\theta$. Adaptive basis functions may be orthonormal by construction, or not. Orthonormality of the basis functions is a nice property, since the total variance is naturally partitioned among the variances of the coefficients:

$$\sum_{i=1}^{N}||y_i-\bar{y}||^2=\sum_{i=1}^{N}\left(\sum_{t=1}^{\mathrm{T}}(y_i(t)-\bar{y}(t))^2\right)\approx\sum_{k=1}^{K}\left(\sum_{i=1}^{N}h_{ik}^2\right)=\sum_{k=1}^{K}||h_k||^2. \tag{3}$$

(Usually, the basis functions are ordered so that the first few capture most of the total variance.) However, even when the basis functions are not orthonormal, the total variance captured by the expansion in terms of the first k ($k\leqslant K$) basis functions can be computed, and orthonormality may be less important than some other features when it comes to sensitivity analysis.

3. Legendre polynomial bases

Since the example is being interpreted as a set of functions of angles from -90° to $+90^\circ$, the Legendre expansion in $\sin(\theta)$ is a natural choice among standard expansions. Fig. 2 shows how the coefficients $\{h_{ik}\}$ of the expansions of the ($N=$) 81 functional outputs depend on the parameters, for $k=1,2,\ldots,6$ ($=K$). The Legendre polynomials are alternately symmetric and anti-symmetric around zero, as shown in the top row of Fig. 2. The first k polynomials define a k-dimensional subspace of the ($T=$) 41-dimensional space in which the output functions are vectors. The percentages at the top show how much of the total variance in the original family of functions lies in this subspace for k up to 6. Note, for future reference, that the six-dimensional subspace defined by the first six polynomials still includes less than 90% of the total variance.

In the second row, the Legendre polynomials are interpreted as perturbations of the overall mean of the 81 output functions. The mean function is the darker line. The mean plus and minus a multiple of the Legendre polynomial are the lighter lines.

The remaining rows contain box plots showing dependencies of the coefficients on the four parameters. Of course, we are not proposing sensitivity analysis by